Simulation of shock-induced chemical reactions in reactive powder mixtures using SPH

Siva Prasad A.V.S. [1], Sumit Basu[1*]
[1] Mechanical Engineering Department, IIT Kanpur, Kalyanpur
Kanpur, UP - 208016, India.

March 24, 2015

Abstract

A completely Lagrangian meshfree numerical model based on Smoothed Particle Hydrodynamics (SPH) is presented to simulate shock-induced chemical reactions (SICR) in reactive powder mixtures. Our numerical model is demonstrated for Nb−Si reaction system.

Keyword: Shock-induced chemical reactions; meshless method; Smoothed Particle Hydrodynamics; reactive powder mixtures.

1 Introduction

Material synthesis by shock compaction of reactive powder mixtures is a very fast process in which the entire sequence of events, starting from shock passage to product formation, occurs in a few microseconds [2]. Numerical simulations, which involve the granular nature of the mixtures, are necessary to understand the possible mechanisms behind these fast reactions. In this work, a 2−D SPH code has been developed to simulate the shock compaction of Nb−Si powder mixture and the formation of $NbSi_2$. Reactions are carried out by defining a distance weighted reaction rate constant with a view of simulating the actual diffusion limited reaction process, without solving the reaction-diffusion equations.

*sbasu@iitk.ac.in

2 Problem description

The problem setup, shown in Fig. 1(a), has a randomly arranged mixture of Nb (light grey) and Si (dark grey) powder particles between two inert walls, which are assumed to be made of high strength steel in this work. The left wall is continuously given an impact velocity, V_0, while the right wall is treated as a non-reflecting boundary. On the top and bottom surfaces, $v_y = 0$ (the velocity in $y-$direction), in order to simulate periodicity of the system in $y-$direction. The equations governing conservation of mass, linear momentum and energy and evolution of species are,

$$\frac{D\rho}{Dt} = -\rho \boldsymbol{\nabla} \cdot \boldsymbol{v},\ \frac{D\boldsymbol{v}}{Dt} = \frac{1}{\rho}\boldsymbol{\nabla} \cdot \boldsymbol{\sigma},\ \frac{De}{Dt} = \frac{1}{\rho}\boldsymbol{\sigma} : \boldsymbol{d} + \dot{Q}_r, \tag{1a}$$

$$-\frac{D}{Dt}N_{\mathrm{n}} = -\frac{1}{2}\frac{D}{Dt}N_{\mathrm{s}} = \frac{D}{Dt}N_{\mathrm{ns}} = \tilde{k}_f\left(r\right) N_{\mathrm{n}} N_{\mathrm{s}}^2, \tag{1b}$$

where, $\boldsymbol{\sigma}$, ρ, $\boldsymbol{d}$, e and $\dot{Q}_r$ are the Cauchy stress tensor, density, the strain rate tensor, the internal energy per unit mass and the net rate of heat generated per unit volume due to the reaction. Also, $\tilde{k}_f\left(r\right)$ is the distance weighted Arrhenius rate constant, N_{n}, N_{s} and N_{ns} are the molar concentrations of Nb, Si and $NbSi_2$. The modified rate constant $\tilde{k}_f\left(r\right)$ is chosen to decay rapidly with distance between Nb and Si material points, r. Mie-Grüneisen equation of state and elastic-viscoplastic constitutive equations are used to describe the deformation behavior of Nb, Si and $NbSi_2$ powder particles [1].

3 Results and discussions

Figures 1(b) and (c) show the contours of $NbSi_2$ mass fraction and the evolution of overall mass fractions of Nb, Si and $NbSi_2$ from simulations carried out at $V_0 = 1250$ m/s. There are unreacted, partially and fully reacted regions in the system, a pattern that is also observed in experiments by [2]. The final overall mass fraction of $NbSi_2$ from our simulation is 0.39, which is in agreement with [2]. The effects of impact speed, initial particle arrangement and mixing ratio (m_r) on the predicted product mass fractions, are shown in Figs. 1(d)$-$(f). The yield of products is maximum within an optimum impact velocity range, while, seems to be weakly dependent on initial particle arrangement of same mixing ratio. However, configurations with stoichiometric and super-stoichiometric mixing ratios improved the product yeild significantly.

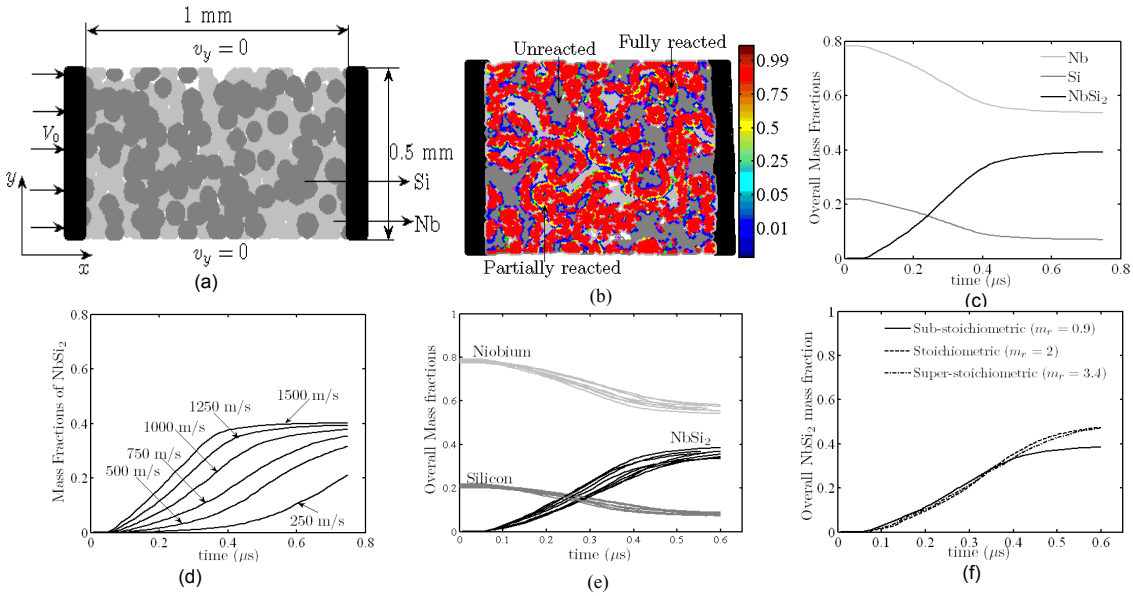

Figure 1: (a) Problem definition, (b) contours of $NbSi_2$ mass fraction, (c) overall mass fractions with time, effects of (d) impact speed, (e) initial particle arrangement and (f) mixing ratio on the predicted mass fractions.

4 Conclusion

A consistent computational procedure to simulate the SICR process is presented. Our numerical model is capable of capturing the physics within acceptable limits of experimental observations.

References

[1] Ian P.H. Do and David J. Benson. Micromechanical modeling of shock-induced chemical reactions in heterogeneous multi-material powder mixtures. *International Journal of Plasticity*, 17:641 – 668, 2001.

[2] K.S. Vecchio, Li-Hsing Yu, and M.A. Meyers. Shock synthesis of Silicides-I. Experimentation and Microstructural evolution. *Acta Metallurgica et Materialia*, 42:701 – 714, 1994.